Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-Principles Simulations of Silicon Nanowires with Different Surface Passivations[1] JUNWEN LI, JOHN W. MINTMIRE, Department of Physics, Oklahoma State University — We report first-principles simulation results for the electronic band structure of silicon nanowires along <100> and <110> directions with different surface passivating groups such as hydrogen, hydroxyl, and methyl within an all-electron, Gaussian type orbital, local density functional approach. We discuss how these different groups affect the band gaps and electron distribution of silicon nanowires. And from the band structures we find that the carrier effective masses of <100>-oriented silicon nanowires exhibit much more dependence on the diameter and passivation compared to those of <110>-oriented nanowires.

[1]This work was supported by the US Department of Energy Grant DE-FG02-07ER46362.

Junwen Li
Department of Physics, Oklahoma State University

Date submitted: 20 Nov 2008 Electronic form version 1.4